Trichloroethylene

79-01-6 | DTXSID0021383

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 94.3 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.67e-01

Confidence level: 5.52e-01

Nearest Neighbors from the Training Set

Image not found
2-Chlorobutane
Measured: 69.0
Predicted: 117

Image not found
2,2-Dimethylpropanoic acid
Measured: 3.50
Predicted: 5.74e-01

Image not found
Propyleneimine
Measured: 820
Predicted: 148

Image not found
Isopropanol
Measured: 197
Predicted: 23.4

Image not found
Triethylfluorosilane
Measured: 3550
Predicted: 24.1